Inverse design of 3d molecular structures with conditional generative neural networks

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Abstract

The rational design of molecules with desired properties is a long-standing challenge in chemistry. Generative neural networks have emerged as a powerful approach to sample novel molecules from a learned distribution. Here, we propose a conditional generative neural network for 3d molecular structures with specified chemical and structural properties. This approach is agnostic to chemical bonding and enables targeted sampling of novel molecules from conditional distributions, even in domains where reference calculations are sparse. We demonstrate the utility of our method for inverse design by generating molecules with specified motifs or composition, discovering particularly stable molecules, and jointly targeting multiple electronic properties beyond the training regime. The targeted discovery of molecules with specific structural and chemical properties is an open challenge in computational chemistry. Here, the authors propose a conditional generative neural network for the inverse design of 3d molecular structures.